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Point Defects in NiAl **S**.A. KAJIHARA, *NRC Associate, Wright Lab.*, C. WOODWARD, *UES, Inc.*, L.H. YANG*, *Lawrence Livermore National Lab.* Ordered intermetallic alloys such as NiAl and TiAl are attractive materials for high temperature applications, but are brittle below about 600 ^{o}C. Experiment has shown that deformation of TiAl is impeded by localized structural defects and impurities. Also, small amounts of ternary additions can have a significant effect on the ductility of NiAl. Local strain fields around point defect centers produce interactions with dislocations which can lead to classical solute hardening and softening. Fundamental studies of the interaction of dislocations and solute atoms improve the understanding of the mechanisms which affect the ductility and strength of these alloys. From this, the effect of composition on structural and deformation properties can be predicted. Using a plane wave basis and norm-conserving pseudopotentials, we investigate vacancy and antisite defects in NiAl. Electronic structure and structural relaxation results are presented.
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